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LIF AND EMISSION STUDIES OF COPPER AND NITROGEN

Final Report

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ABSTRACT

A technique is developed to determine the rotational temperature of Nitrogen Molecular Ion (N_2^+) from the emission spectra of B-X transition, when P and R branches are not resolved. Its validity is tested on simulated spectra of the 0-1 band of N_2^+ produced under low resolution. The method is applied to experimental spectra of N_2^+ taken in the shock layer of a blunt body at distances of 1.91 cm, 2.54 cm, and 3.18 cm from the body.

The laser induced fluorescence (LIF) spectra of copper atoms is analyzed to obtain the free stream velocities and temperatures. The only broadening mechanism considered is Doppler broadening. The temperatures are obtained by manual curve fitting; and the results are compared with least square fits. The agreement on the average is within 10%.

INTRODUCTION

There is a strong need for non-intrusive diagnostic techniques such as passive radiation techniques which utilize radiation emitted by the plasma or active radiation techniques such as Laser Induced fluorescence (LIF) measurements. These techniques are essential to the arc jet flow studies in order to fully understand the nonequilibrium flow conditions spacecraft encounter during reentry. The arc jet facilities simulate the spacecraft reentry conditions and are used for testing thermal protection materials. The identification, characterization, velocity and temperature determination of different atomic, molecular and ionic species makes an important contribution to the arc jet flow studies. The major species of interest in the spacecraft reentry flow environment are N_2 , O_2 , NO , N_2^+ , N , O , O_2^+ , NO^+ , N^+ , O^+ and electrons. Concentration of these species change when the enthalpy of the flow changes. This report is divided into two parts, one on the analyses of the emission spectra and the other on the analysis of the LIF data.

Emission studies: During the last couple of years the arc jet flow diagnostic program at NASA, Johnson Space Center reported emission studies (Ref.1 and 2) of N_2 and N_2^+ for vibrational and rotational temperature determination across the shock layer. This technique involves calculating the spectrum for a number of cases and obtain integrals over the wavelength regions of the spectrum as a function of temperature. Ratios of these integrals were then related to the temperatures used to generate the spectra. Spectral integrals from the measured spectra are then compared with the calculated values to determine the temperature. This technique has some limitations and requires numerous parameters to produce the calculated spectra. This method requires repetitive calculations be performed each time a comparison is made. In this report a simpler technique is presented to find the rotational temperatures of N_2^+ in the shock layer. This can be applied to other molecules as well.

LIF studies: The LIF measurements reported here probe different species with a known excitation mechanism using selective excitation with a narrow band laser. Preliminary LIF studies of copper are used to calculate the velocity and temperature are presented here.

MEASUREMENTS

Emission spectra: Details of the experimental set up to record the emission spectrum of nitrogen in the wavelength region of 340 nm to 480 nm are reported earlier (Ref.3).

LIF studies on copper: Laser fluorescence spectra of copper recorded earlier using the experimental setup shown in Fig.1, are analyzed. The setup essentially consists of a YAG pumped dye laser system with intracavity etalons in the dye as well as in the pump laser reducing the dye fundamental band width to less than 0.08 cm^{-1} . To probe the copper atoms, Dicyanomethylene (DCM) dye is used together with a KD*P doubling crystal to produce laser light at 327.5 nm. Details of the laser fluorescence detection and control electronics along with laser pulse energy used for copper are reported earlier (Ref.4). Velocity measurements of the free stream for various mass flow rates and arc currents have been carried out using copper as the tracer material. The excitation wavelength is about 327.5 nm (Figs. 2) and the 578 nm fluorescence is collected at right angles to the flow using cutoff and narrow band interference filters. Two separate measurements were taken for Doppler shift studies one with the laser beam perpendicular and the other at an angle of 60° with respect to the flow direction.

RESULTS AND ANALYSIS

Emission spectra of N_2^+ : The rotational structure of the 0-1 band of B-X transition of N_2^+ is shown in Fig. 3. Due to the limited resolution the P and R branches are not resolved. In order to analyze and determine the rotational temperature, we have developed a method described in an earlier report (Ref.3). For completeness of this report the equations are shown in Appendix 1 and 2. In order to test the accuracy of these equations, simulated spectra of N_2^+ using NEQAIR program under low resolution are produced at various temperatures. A sample spectra produced at 8000 K is shown in Fig. 4. We have now used the areas and corrected them for P and R branches using equations (7) and (8) shown in Appendix 2., at various temperatures (T). Graphs are now plotted: $\ln [I_{PC}/(k'+k''+1)]$ against $k'(k'+1)$ for P-branch and $\ln [I_{RC}/(k'+k''+1)]$ against $k'(k'+1)$ for R-branch. According to equation (4) shown in Appendix 1, as given by Herzberg (Ref.5), the slope of the line gives $B_0 hC/KT$ from which the rotational temperature can be determined. The temperatures (T_P and T_R) are now calculated using the slopes of the straight lines obtained from the graphs for both P and R branches. The particular set for which the temperature $T_P = T_R = T$ is considered as the rotational temperature. Fig. 5 is a graph showing the agreement between P and R branches at 8000 K. Table 1 shows the temperatures calculated using the slopes of the lines at three different temperatures.

This method is now applied to the spectra taken on February '89 at 1.91 cm, 2.54 cm and 3.18 cm positions in the shock layer of a blunt body. Figs. 6 and 7 shows the graphs plotted for corrected P and R branch intensities taking the areas and the results are tabulated in Table - 2.

The calculated temperatures are slightly less than the temperatures obtained by Blackwell et al. (Ref. 4) using computer simulation techniques. This low temperature seems to be due to the overlap of intensity of some other bands of the same species or due to the emissions of the species present in the shock layer in the region analyzed. If an account can be made for this background intensity rotational temperatures can be more precisely determined even in unresolved bands. Work in this direction will be continued in the future.

LIF studies on copper: A representative spectrum of Doppler shifted copper spectrum is shown in Fig. 8. The measured Doppler profiles are used to determine the velocity and temperature. The velocity is obtained using the relation

$$V = C \Delta W / W_0 \quad (1)$$

where V is the velocity of the free stream, C is the speed of light, W is the measured Doppler shift and W_0 is the laser excitation frequency. A graph of the measured velocity against bulk enthalpy is shown in Fig. 9 and it demonstrates the expected increase in velocity with increasing enthalpy.

To determine the temperature, a linear curve fit of the quadruplet of Gaussian profiles was fit to the measured profiles. The laser line width was accounted for by folding its profile with the Doppler profile. Both were taken to be Gaussian.

The intensity of Gaussian line shape is given by

$$I(W) = I_0 \exp[-4 \ln 2 (W_0 - W / \Delta W_D)^2] \quad (2)$$

and the Doppler Width ΔW_D is given by

$$\Delta W_D = W_0 / C (8 RT \ln 2 / M)^{1/2}$$

where

- I_0 = the peak intensity of the Doppler profile
- W_0 = the frequency at peak intensity
- R = gas constant
- T = Temperature in Kelvin
- M = Mass of copper atom.

Fitted curves at different temperatures are developed using equation (2) and were overlapped on the experimental curve. The one that best fits to the experimental curve is taken to be the temperature at that flow rate. A sample curve fit using one of the two peaks is shown in Fig. 10. The first peak is saturated and so only one peak is considered for an accurate determination of the temperature. Temperatures are determined using this method at various flow rates and the results are presented in Table - 3. The results do not

compare particularly well with the least square fit, indicating the assumptions used in the simple calculations are not adequate. More systematic study has to be carried out and using least square fit Gaussian profiles may yield a more precise temperature determination. It may be noted that a Voigt profile (a combination of Gaussian and Lorentzian profile) may be the appropriate choice for future studies.

CONCLUSIONS

On the basis of the analysis made in both the projects the following conclusions are made:

1. Rotational temperature measurements can be made within 5% even in the case of unresolved bands due to a single species if there is no overlap of other bands.
2. This method can be extended to the observed experimental spectra, where other species are present provided the contribution due to the background is accounted for.
3. The method used to find the temperature of Doppler shifted curves in copper agrees on the average with in 10% with that obtained using least square fit. The velocity can be calculated to an accuracy of 10%.

ACKNOWLEDGMENTS

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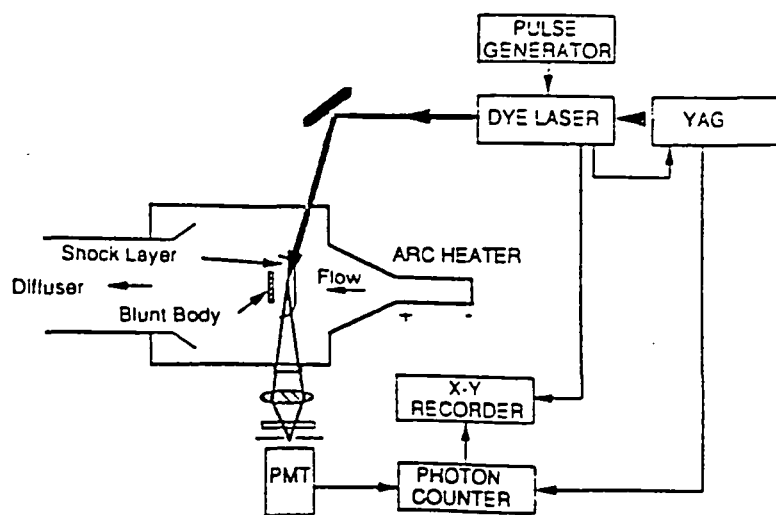


Fig. 1 Experimental setup

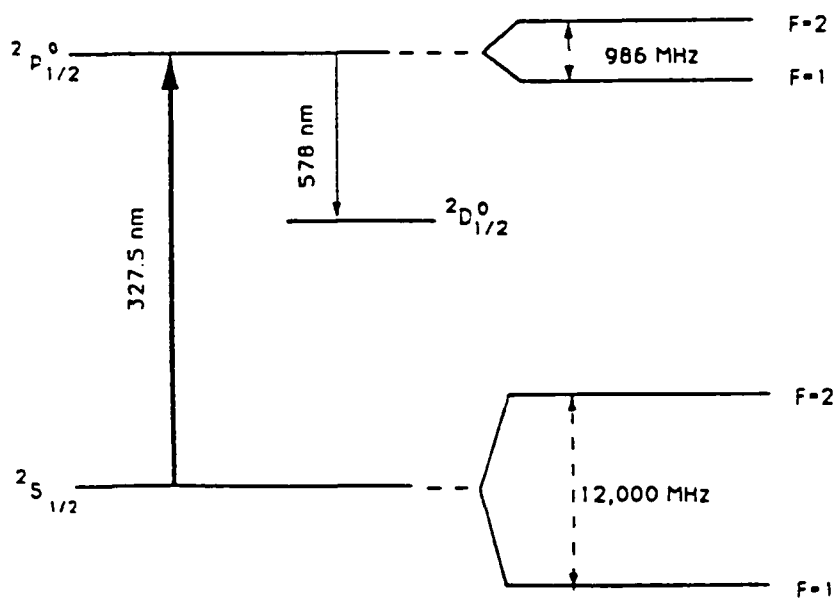


Fig. 2. Detailed energy level diagram of copper atom

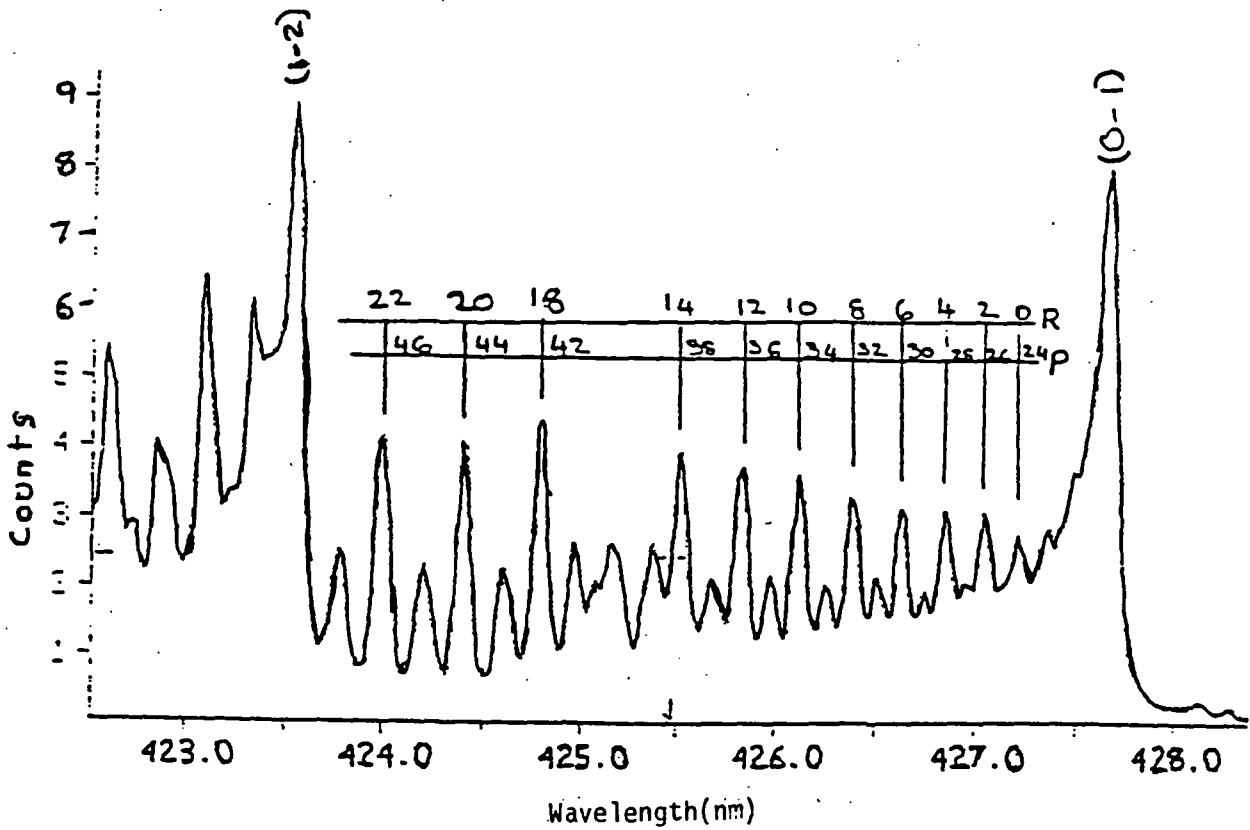


Figure 3.- 0-1 band of N_2^+ B-X system -low resolution

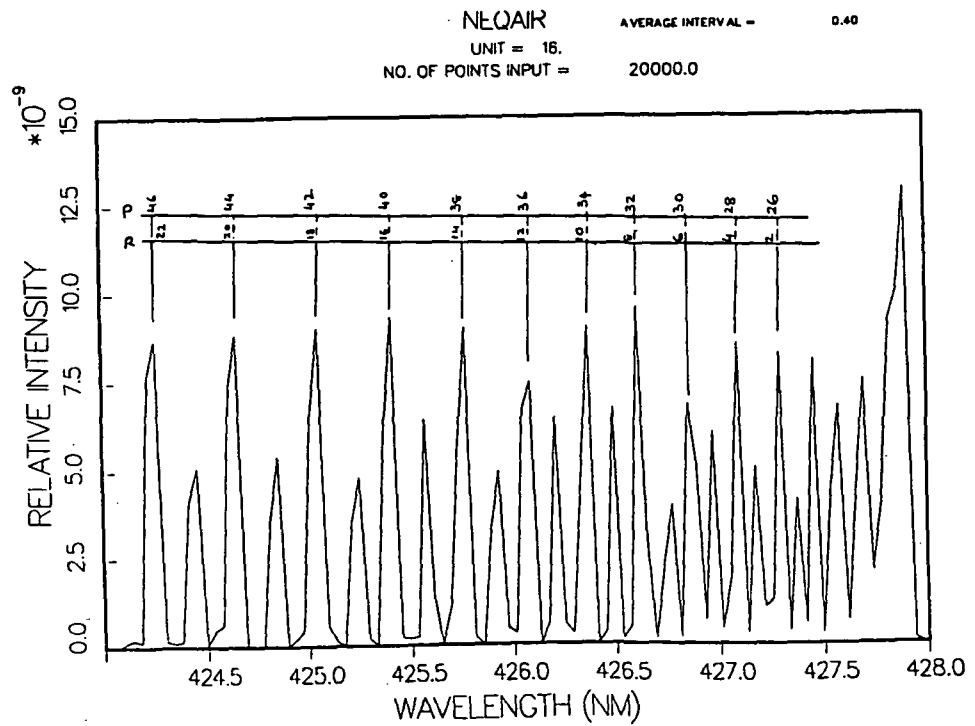


Figure 4.-simulated low resolution spectrum of 0-1 band of N_2^+ simulated spectra,8000K

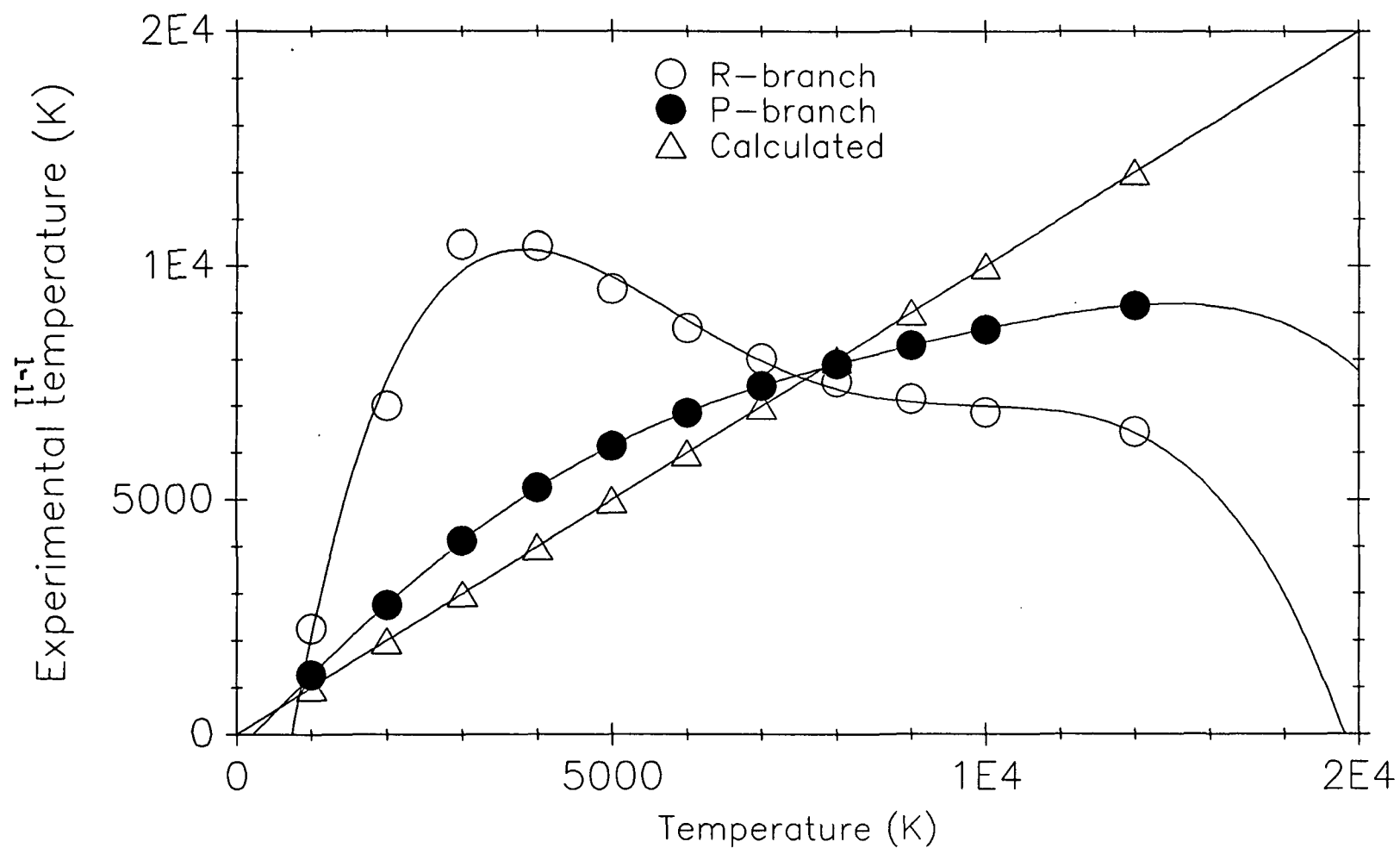


Figure 5.—Rotational temperature of nitrogen molecular ion
—simulated spectra, (8000K)

Nitrogen Molecular Ion (0,1)band,3.18cm,600amp
P-branch

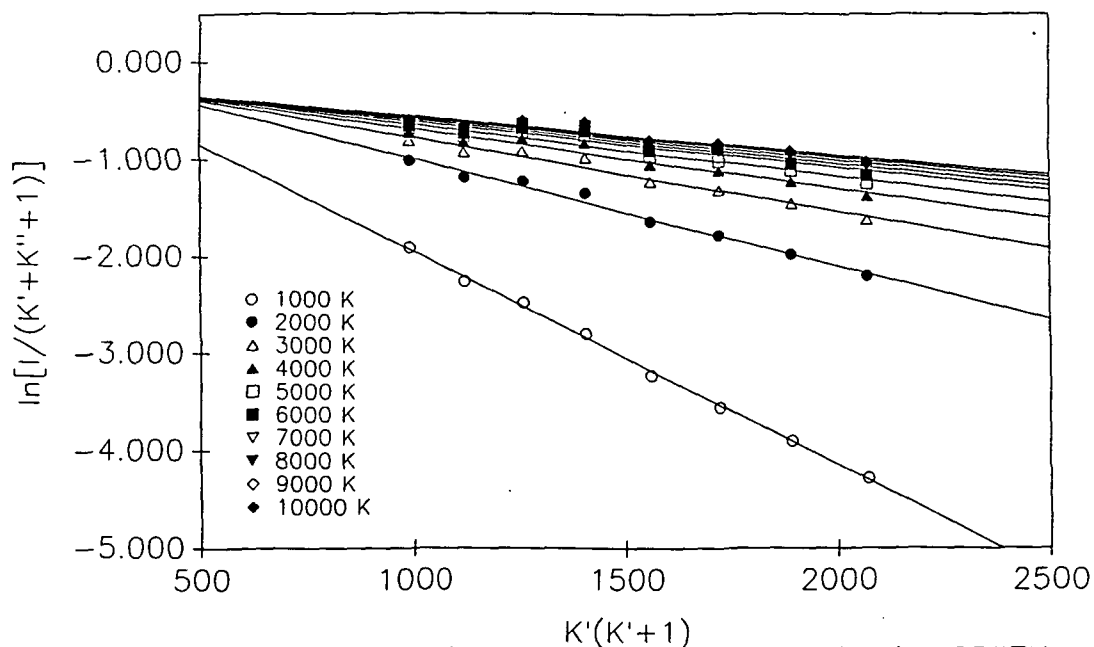


Figure 6.-Rotational temperature determination,6337K

Nitrogen Molecular Ion(0,1)band,3.18cm,600amp
R-branch

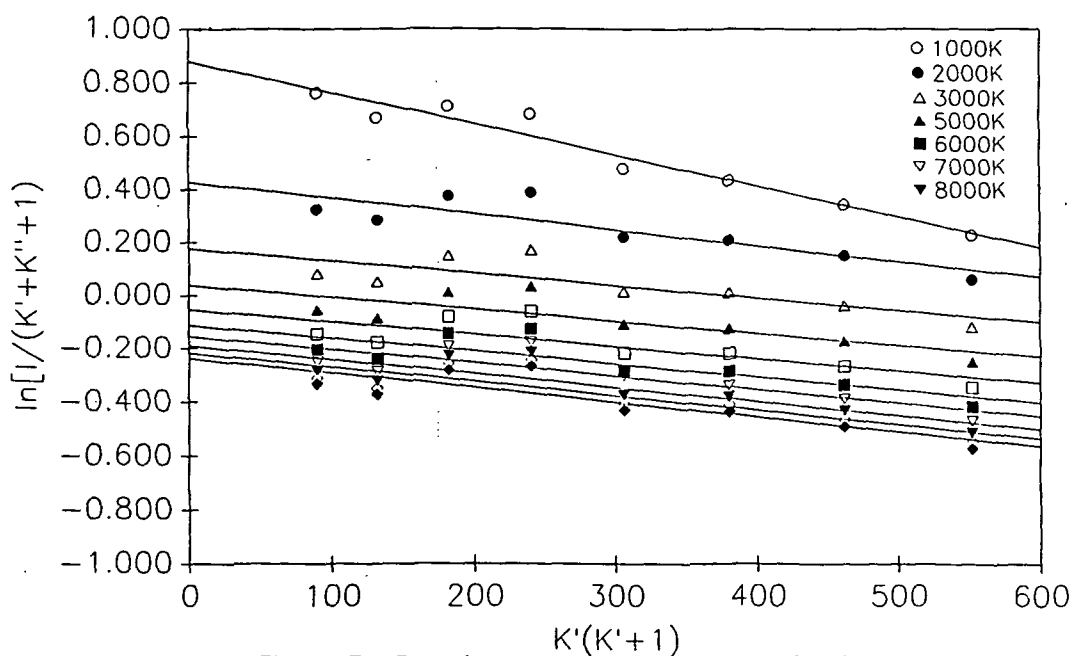


Figure 7.-Rotational temperature determination,6131K

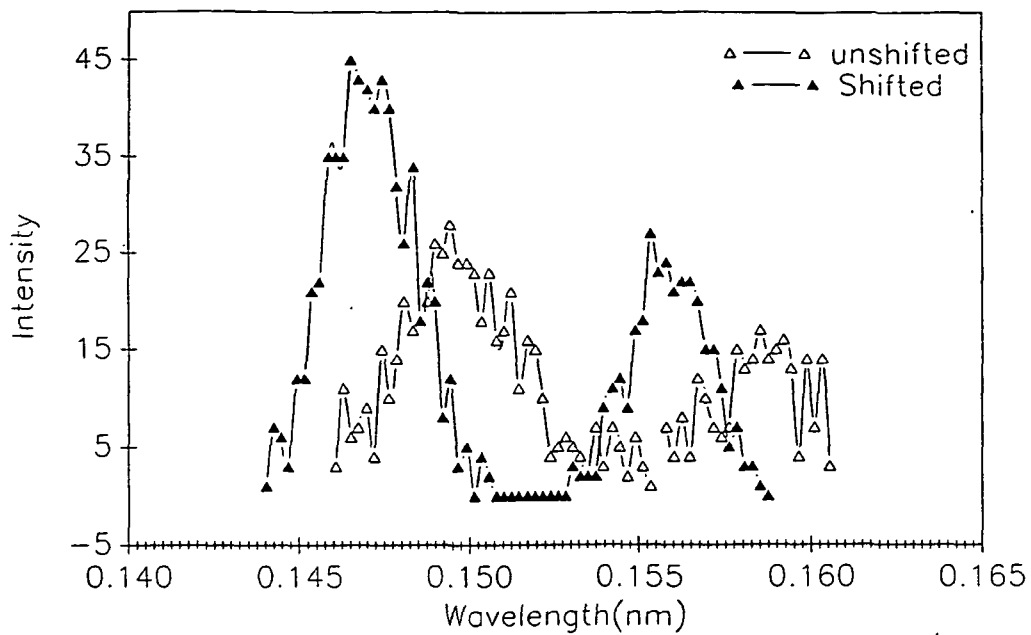


Figure 8.-Copper Doppler shift measurements,700A,0.15lb/s

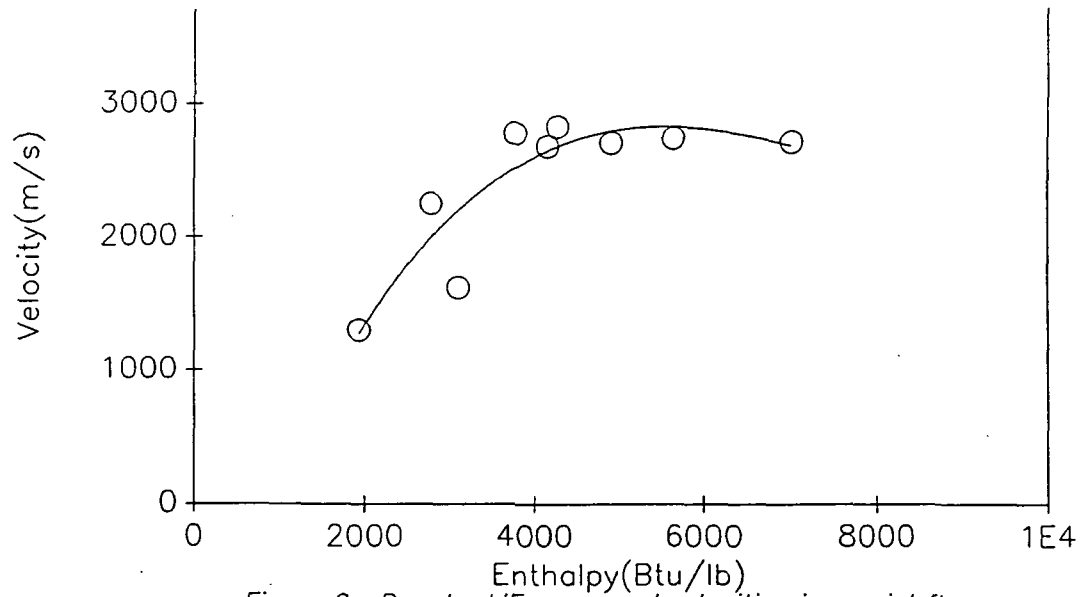


Figure 9.-Doppler LIF measured velocities in arc jet flows

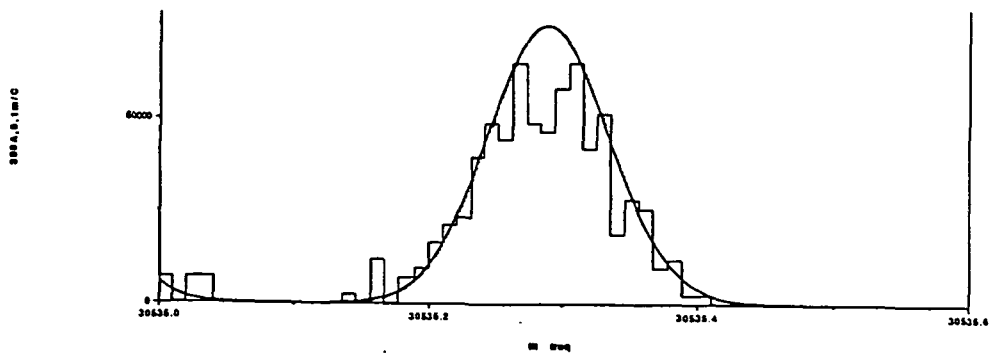


Figure 10.-Copper LIF spectrum and curve fit,300A,0.01lb/s,1100K

TABLE 1.- SIMULATION SPECTRA - COMPARISON

T (K)	T _P (K)	% Error	T _P (K)	% Error
8000	7906	1.1	7553	5.8
6000	6234	3.9	6388	6.5
3000	3125	4.2	3217	7.2

TABLE 2.- ROTATIONAL TEMPERATURES OF SHOCK LAYER

Position of Shock layer (cm)	T _P (K)	% Error	T _P (K)	% Error
1.91	3991	0.4	3982	0.2
2.54	2954	1.5	3045	1.5
3.18	6337	5.0	6131	2.2

TABLE 3.- COPPER DOPPLER SHIFT DATA

Current (Amps)	Flow Rate (lb/s)	Doppler Shift 10 ⁻³ nm	Velocity (m/s)	Temp (K)	Enthalpy (Btu/lb)
				Curve fit	least Square fit
700	0.05	1.486	2721	--	--
	0.10	1.500	2747	--	2022
	0.15	1.480	2711	1200	1148
	0.20	1.468	2688	1500	1486
	0.25	1.519	2782	--	1076
500	0.10	1.547	2834	1400	1457
	0.20	0.885	1621	1300	1478
300	0.10	1.232	2256	1100	1117
	0.20	0.709	1299	600	498

ROTATIONAL TEMPERATURE EQUATIONS

$$I(\text{P - Branch}) = A - 2J e^{-\frac{B_0 J(J-1)hc}{kT}} \quad (1)$$

$$I(\text{R - branch}) = A - 2(J+1) e^{-\frac{B_0 (J+1)(J+2)hc}{kT}} \quad (2)$$

Rearranging equations (1) and (2)

$$\ln \left[\frac{I_p}{2J} \right] = \ln A - \frac{B_0 J(J-1)hc}{kT}$$

$$\ln \left[\frac{I_p}{2J} \right] = A' - \frac{B_0 J(J-1)hc}{kT} \quad (3)$$

Similarly for R Branch

$$\ln \left[\frac{I_R}{2(J+1)} \right] = A' - \frac{B_0 (J+1)(J+2)hc}{kT} \quad (4)$$

Equation (3) and (4) can general be written for either case as

$$\ln \left[\frac{I}{k' + k'' + 1} \right] = A - \frac{B' K' (k' + 1)hc}{kT}$$

where k' - upper rotational state quantum number
 k'' - lower rotational state quantum number

CORRECTED INTENSITIES

$$I_{\text{EXP}} = I_{\text{P}} + I_{\text{R}} \quad (5)$$

$$\frac{I_{\text{EXP}}}{I_{\text{R}}} = \frac{I_{\text{P}}}{I_{\text{R}}} + 1 \quad (6)$$

Let $\frac{I_{\text{P}}}{I_{\text{R}}} = B$ where I_{P} and I_{R} are the intensities calculated for any temperature using equations (1) and (2)

$$I_{\text{Rc}} = I_{\text{EXP}} \left[\frac{1}{1 + B} \right] \quad (7)$$

$$I_{\text{Pc}} = I_{\text{EXP}} \left[\frac{1}{1 + \frac{1}{B}} \right] \quad (8)$$

I_{Rc} and I_{Pc} are the intensity contributions of P and R branches in the observed spectra